

Tight Binding parameters of GaAs and MgO

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TABLE I: Tight Binding Parameters for bulk GaAs

Parameter	value	Parameter	value
E_{sa}	-4.5863	$s_a^* p_c \sigma$	2.6877
E_{pa}	1.4694	$s_c^* p_a \sigma$	1.8335
E_{s^*a}	10.0480	$s_a d_c \sigma$	-2.1172
E_{da}	11.2878	$s_c d_a \sigma$	-2.9128
E_{sc}	-1.3323	$s_a^* d_c \sigma$	-0.4974
E_{pc}	9.5885	$s_c^* d_a \sigma$	-2.9971
E_{s^*c}	25.6752	$pp\sigma$	3.8065
E_{dc}	35.2863	$pp\pi$	-1.5010
Δ_a	0.1259	$p_a d_c \sigma$	-1.2077
Δ_c	0.1235	$p_c d_a \sigma$	-1.9855
$ss\sigma$	-1.7615	$p_a d_c \pi$	3.1547
$s^* s^* \sigma$	-0.8374	$p_c d_a \pi$	2.3234
$s_a^* s_c \sigma$	-1.1173	$dd\sigma$	-1.9986
$s_a s_c^* \sigma$	-2.9313	$dd\pi$	3.1681
$s_a p_c \sigma$	2.1768	$dd\delta$	-2.3137
$s_c p_a \sigma$	3.6705		

TABLE II: Tight Binding Parameters for bulk MgO

Parameter	Value	Parameter	Value
E_{sa}	-7.1496	$p_a d_c \pi$	1.5284
E_{pa}	5.8926	$p_c d_a \pi$	-4.0453
E_{s^*a}	23.8138	$d_a d_c \sigma$	-1.0038
E_{da}	40.0285	$d_a d_c \pi$	5.0830
E_{sc}	38.4754	$d_a d_c \delta$	-0.6323
E_{pc}	32.1465	$s_a s_a \sigma$	-0.2718
E_{s^*c}	45.5084	$s_a^* s_a^* \sigma$	-0.4690
E_{dc}	57.9865	$s_a s_a^* \sigma$	-0.0001
Δ_a	0.0031	$s_a p_a \sigma$	0.3388
Δ_c	0.0298	$s_a^* p_a \sigma$	0.1965
$s_a s_c \sigma$	-0.1192	$s_a d_a \sigma$	-0.3380
$s_a^* s_c^* \sigma$	1.6477	$s_a^* d_a \sigma$	-0.4407
$s_a^* s_c \sigma$	-0.6008	$p_a p_a \sigma$	0.4371
$s_a s_c^* \sigma$	-0.6347	$p_a p_a \pi$	-0.0641
$s_a p_c \sigma$	-2.0013	$p_a d_a \sigma$	-0.4039
$s_c p_a \sigma$	0.3283	$p_a d_a \pi$	0.6986
$s_a^* p_c \sigma$	2.1584	$d_a d_a \sigma$	-2.3768
$s_c^* p_a \sigma$	2.1282	$d_a d_a \pi$	0.4556
$s_a d_c \sigma$	0.6641	$d_a d_a \delta$	0.0967
$s_c d_a \sigma$	-2.9483		
$s_a^* d_c \sigma$	1.6890		
$s_c^* d_a \sigma$	3.1534		
$p_a p_c \sigma$	0.1743		
$p_a p_c \pi$	-0.4703		
$p_a d_c \sigma$	-1.9960		
$p_c d_a \sigma$	0.0519		